

Safety data sheet

Safe Work Australia - Code of Practice



Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: **6889**
Version: **GHS 2.0 en**
Replaces version of: 2016-01-13
Version: (GHS 1)

date of compilation: 2016-01-13
Revision: 2019-07-03

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

Identification of the substance	Isooctane
Article number	6889
Registration number (REACH)	01-2119457965-22-xxxx
Index No	601-009-00-8
EC number	208-759-1
CAS number	540-84-1

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses: laboratory chemical
laboratory and analytical use

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

Telephone: +49 (0) 721 - 56 06 0
Telefax: +49 (0) 721 - 56 06 149
e-mail: sicherheit@carlroth.de
Website: www.carlroth.de

Competent person responsible for the safety data sheet : Department Health, Safety and Environment

e-mail (competent person) : sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 Westmead, NSW	131126	

Emergency information service

Poison Centre Munich: +49/(0)89 19240

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

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Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
2.6	flammable liquid	(Flam. Liq. 2)	H225
3.1D	acute toxicity (dermal)	(Acute Tox. 5)	H313
3.1I	acute toxicity (inhal.)	(Acute Tox. 5)	H333
3.2	skin corrosion/irritation	(Skin Irrit. 2)	H315
3.8D	specific target organ toxicity - single exposure (narcotic effects, drowsiness)	(STOT SE 3)	H336
3.10	aspiration hazard	(Asp. Tox. 1)	H304
4.1A	hazardous to the aquatic environment - acute hazard	(Aquatic Acute 1)	H400
4.1C	hazardous to the aquatic environment - chronic hazard	(Aquatic Chronic 1)	H410

The most important adverse physicochemical, human health and environmental effects

Narcotic effects.

2.2 Label elements

Labelling GHS

Signal word

Danger

Pictograms

GHS02, GHS07,
GHS08, GHS09



Hazard statements

H225 Highly flammable liquid and vapour
H304 May be fatal if swallowed and enters airways
H313+H333 May be harmful in contact with skin or if inhaled
H315 Causes skin irritation
H336 May cause drowsiness or dizziness
H410 Very toxic to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

Precautionary statements - response

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P302+P352 IF ON SKIN: Wash with plenty of soap and water.
P331 Do NOT induce vomiting.
P370+P378 In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction.

Precautionary statements - storage

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P403+P233
P403+P235

Store in a well-ventilated place. Keep container tightly closed.
Store in a well-ventilated place. Keep cool.

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)



H304
H313+H333

May be fatal if swallowed and enters airways.
May be harmful in contact with skin or if inhaled.

P301+P310
P331

IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
Do NOT induce vomiting.

2.3 Other hazards

There is no additional information.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	2,2,4-Trimethylpentane
Index No	601-009-00-8
Registration number (REACH)	01-2119457965-22-xxxx
EC number	208-759-1
CAS number	540-84-1
Molecular formula	C ₈ H ₁₈
Molar mass	114.2 g/mol

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In case of skin irritation, consult a physician.

Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

Following ingestion

Rinse mouth. Do not induce vomiting. Observe aspiration hazard if vomiting occurs. Call a physician immediately.

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4.2 Most important symptoms and effects, both acute and delayed

Following inhalation: Drowsiness, Dizziness, Narcosis,
Following skin contact: Irritation,
After eye contact: Irritant effects,
After ingestion: Aspiration hazard

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings
water spray, foam, dry extinguishing powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours can form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: carbon monoxide (CO), carbon dioxide (CO₂)

5.3 Advice for firefighters

Do not allow firefighting water to enter drains or water courses. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus. Beware of reignition.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Use personal protective equipment as required. Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it. Explosive properties.

6.3 Methods and material for containment and cleaning up

Advices on how to contain a spill

Covering of drains.

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Advices on how to clean up a spill

Absorb with liquid-binding material (e.g. sand, diatomaceous earth, acid- or universal binding agents).

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation. Use extractor hood (laboratory). Avoid: Aerosol or mist formation.

• Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge. Due to danger of explosion, prevent leakage

of vapours into cellars, flues and ditches.

• Measures to protect the environment

Avoid release to the environment.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs. When using do not smoke.

7.2 Conditions for safe storage, including any incompatibilities

Store in a well-ventilated place. Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice

Ground/bond container and receiving equipment.

• Ventilation requirements

Use local and general ventilation.

• Specific designs for storage rooms or vessels

Recommended storage temperature: 15 – 25 °C.

7.3 Specific end use(s)

No information available.

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SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Data are not available.

Relevant DNELs/DMELs/PNECs and other threshold levels

• human health values

Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	2,035 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	773 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



• hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

• type of material

NBR (Nitrile rubber)

• material thickness

>0,3 mm

• breakthrough times of the glove material

>480 minutes (permeation: level 6)

• other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Flame-retardant protective clothing.

Respiratory protection



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Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C , colour code: Brown).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance

Physical state	liquid (fluid)
Colour	colourless
Odour	like: Gasoline
Odour threshold	No data available

Other physical and chemical parameters

pH (value)	(neutral)
Melting point/freezing point	-107 °C
Initial boiling point and boiling range	99 °C at 1,013 hPa
Flash point	-12 °C (closed cup)
Evaporation rate	no data available
Flammability (solid, gas)	not relevant (fluid)
<u>Explosive limits</u>	
• lower explosion limit (LEL)	1 vol% (45 g/m ³)
• upper explosion limit (UEL)	6 vol% (290 g/m ³)
Explosion limits of dust clouds	not relevant
Vapour pressure	53 hPa at 20 °C
Density	0.69 g/cm ³ at 15 °C
Vapour density	3.9 (air = 1)
Bulk density	Not applicable
Relative density	Information on this property is not available.
<u>Solubility(ies)</u>	
Water solubility	2.2 mg/l at 25 °C
<u>Partition coefficient</u>	
n-octanol/water (log KOW)	4.08 (ECHA)
Soil organic carbon/water (log KOC)	2.381 (ECHA)
Auto-ignition temperature	418 °C - ECHA
Decomposition temperature	no data available
Viscosity	
• kinematic viscosity	0.7246 mm ² /s

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• dynamic viscosity	0.5 mPa s at 20 °C
Explosive properties	Shall not be classified as explosive
Oxidising properties	none

9.2 Other information

Surface tension	18.77 mN/m (20 °C)
Refractive index	1.392

SECTION 10: Stability and reactivity

10.1 Reactivity

Risk of ignition. Vapours can form explosive mixtures with air.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: Strong oxidiser

10.4 Conditions to avoid

UV-radiation/sunlight. Keep away from heat.

10.5 Incompatible materials

different plastics

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Exposure route	Endpoint	Value	Species	Source
oral	LD50	>5,000 mg/kg	rat	ECHA
inhalation: vapour	LC50	>33.52 mg/l/4h	rat	ECHA
dermal	LD50	>2,000 mg/kg	rabbit	ECHA

Skin corrosion/irritation

Causes skin irritation.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor as a reproductive toxicant

• Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

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- **Specific target organ toxicity - repeated exposure**

Shall not be classified as a specific target organ toxicant (repeated exposure).

- **Aspiration hazard**

May be fatal if swallowed and enters airways.

Symptoms related to the physical, chemical and toxicological characteristics

- **If swallowed**

vomiting, aspiration hazard

- **If in eyes**

causes slight to moderate irritation

- **If inhaled**

drowsiness, dizziness, narcosis

- **If on skin**

causes skin irritation

- **Other information**

None

SECTION 12: Ecological information

12.1 Toxicity

Very toxic to aquatic life with long lasting effects.

Aquatic toxicity (acute)

Very toxic to aquatic organisms.

Endpoint	Value	Species	Source	Exposure time
LC50	0.11 mg/l	fish	ECHA	96 h
EC50	0.4 mg/l	aquatic invertebrates	ECHA	48 h

Aquatic toxicity (chronic)

May cause long-term adverse effects in the aquatic environment.

Endpoint	Value	Species	Source	Exposure time
EC50	0.23 mg/l	aquatic invertebrates	ECHA	21 d
NOEC	0.17 mg/l	aquatic invertebrates	ECHA	21 d

12.2 Process of degradability

Theoretical Oxygen Demand: 3.501 mg/mg

Theoretical Carbon Dioxide: 3.082 mg/mg

Process	Degradation rate	Time
oxygen depletion	61.81 %	70 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

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n-octanol/water (log KOW)	4.08
BCF	231 (ECHA)

12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	2.381
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12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains. Avoid release to the environment. Refer to special instructions/safety data sheets.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

Sewage disposal-relevant information

Do not empty into drains. Avoid release to the environment. Refer to special instructions/safety data sheets.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.


13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions.

SECTION 14: Transport information

14.1 UN number	1262
14.2 UN proper shipping name	OCTANES
Hazardous ingredients	Isooctane
14.3 Transport hazard class(es)	
Class	3 (flammable liquids)

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|------|-----------------------|---|
| 14.4 | Packing group | II (substance presenting medium danger) |
| 14.5 | Environmental hazards | hazardous to the aquatic environment |

14.6 Special precautions for user

Provisions for dangerous goods (ADR) should be complied within the premises.

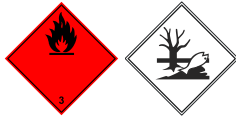
14.7 Transport in bulk according to Annex II of MARPOL and the IBC Code

The cargo is not intended to be carried in bulk.

14.8 Information for each of the UN Model Regulations

• Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)

UN number	1262
Proper shipping name	OCTANES
Particulars in the transport document	UN1262, OCTANES, 3, II, (D/E), environmentally hazardous
Class	3
Classification code	F1
Packing group	II
Danger label(s)	3 + "fish and tree"



Environmental hazards	yes (hazardous to the aquatic environment)
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
Transport category (TC)	2
Tunnel restriction code (TRC)	D/E
Hazard identification No	33
Emergency Action Code	3YE

• International Maritime Dangerous Goods Code (IMDG)

UN number	1262
Proper shipping name	OCTANES
Particulars in the shipper's declaration	UN1262, OCTANES, 3, II, -12°C c.c., MARINE POLLUTANT
Class	3
Marine pollutant	yes (P) (hazardous to the aquatic environment)
Packing group	II
Danger label(s)	3 + "fish and tree"



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Special provisions (SP)	-
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
EmS	F-E, S-E
Stowage category	B
• International Civil Aviation Organization (ICAO-IATA/DGR)	
UN number	1262
Proper shipping name	Octanes
Particulars in the shipper's declaration	UN1262, Octanes, 3, II
Class	3
Environmental hazards	yes (hazardous to the aquatic environment)
Packing group	II
Danger label(s)	3



Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

National inventories

Substance is listed in the following national inventories:

Country	National inventories	Status
AU	AICS	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed

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Country	National inventories	Status
US	TSCA	substance is listed

Legend

AICS	Australian Inventory of Chemical Substances
CICR	Chemical Inventory and Control Regulation
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

16.1 Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.1		Classification acc. to GHS: change in the listing (table)	yes
2.1	Remarks: For full text of Hazard- and EU Hazard-statements: see SECTION 16.		yes
2.2		Pictograms: change in the listing (table)	yes
2.2		Hazard statements: change in the listing (table)	yes
2.2		Precautionary statements - prevention: change in the listing (table)	yes
2.2		Precautionary statements - response: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
8.1	Occupational exposure limit values (Workplace Exposure Limits): not relevant	Occupational exposure limit values (Workplace Exposure Limits): Data are not available.	yes
8.1		• human health values: change in the listing (table)	yes
14.2	Hazardous ingredients: ISOCTANE ROTIPURAN® ≥ 99%, p.a., ACS	Hazardous ingredients: Isooctane	yes
14.3	Transport hazard class(es)	Transport hazard class(es): class 3 hazard - flammable liquids	yes

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Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
14.8	Particulars in the transport document: UN1262, OCTANES, (2,2,4-trimethylpentane), 3, II, (D/E), environmentally hazardous	Particulars in the transport document: UN1262, OCTANES, 3, II, (D/E), environmentally hazardous	yes
14.8		Emergency Action Code: 3YE	yes
14.8	Particulars in the shipper's declaration: UN1262, OCTANES, (2,2,4-trimethylpentane), 3, II, -12°C c.c., MARINE POLLUTANT	Particulars in the shipper's declaration: UN1262, OCTANES, 3, II, -12°C c.c., MARINE POLLUTANT	yes
14.8	Marine pollutant: yes (hazardous to the aquatic environment)	Marine pollutant: yes (P) (hazardous to the aquatic environment)	yes
14.8		• International Civil Aviation Organization (ICAO-IATA/DGR)	yes
14.8		UN number: 1262	yes
14.8		Proper shipping name: Octanes	yes
14.8		Particulars in the shipper's declaration: UN1262, Octanes, 3, II	yes
14.8		Class: 3	yes
14.8		Environmental hazards: yes (hazardous to the aquatic environment)	yes
14.8		Packing group: II	yes
14.8		Danger label(s): 3	yes
14.8		Danger label(s): change in the listing (table)	yes
14.8		Excepted quantities (EQ): E2	yes
14.8		Limited quantities (LQ): 1 L	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
BCF	bioconcentration factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DGR	Dangerous Goods Regulations (see IATA/DGR)
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
EINECS	European Inventory of Existing Commercial Chemical Substances

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Abbr.	Descriptions of used abbreviations
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
index No	the Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
vPvB	very Persistent and very Bioaccumulative

Key literature references and sources for data

- UN Recommendations on the Transport of Dangerous Good
- Dangerous Goods Regulations (DGR) for the air transport (IATA)
- International Maritime Dangerous Goods Code (IMDG)

List of relevant phrases (code and full text as stated in chapter 2 and 3)

Code	Text
H225	highly flammable liquid and vapour
H304	may be fatal if swallowed and enters airways
H313	may be harmful in contact with skin
H315	causes skin irritation
H333	may be harmful if inhaled
H336	may cause drowsiness or dizziness
H400	very toxic to aquatic life
H410	very toxic to aquatic life with long lasting effects

Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.